

How and why to think about scattering in terms of wave packets instead of plane waves

Travis Norsen, Joshua Lande
Marlboro College
Marlboro, VT 05344

S. B. McKagan
JILA, University of Colorado and NIST
Boulder, CO, 80309
 (Dated: April 17, 2009)

We discuss “the plane wave approximation” to quantum mechanical scattering using simple one-dimensional examples. Our central claims are that (a) the plane waves of standard calculations can and should be thought of as very wide wave packets, and (b) the calculations of reflection and transmission probabilities R and T in standard textbook presentations involve an approximation which is almost never discussed. We present a simple and intuitively revealing alternative way to derive and understand the connection between asymptotic wave function amplitudes and scattering probabilities, which also has the benefit of bringing the approximate character of standard plane wave calculations out into the light. We then develop an under-appreciated exact expression for scattering probabilities, using it to calculate, for two standard examples, expressions for R and T for an incident wave packet. Comparing these results to the corresponding probabilities calculated using the plane wave approximation helps illuminate the domain of applicability of that approximation and thus underscores the importance of thinking about scattering in terms of wave packets instead of plane waves.

I. INTRODUCTION

Scattering is arguably the most important topic in quantum physics. Virtually everything we know about the micro-structure of matter, we know from scattering experiments. And so the theoretical techniques involved in predicting and explaining the results of these experiments play a justifiably central role in quantum physics courses at all levels in the physics curriculum, from Modern Physics for sophomores through Quantum Field Theory for graduate students.

Given the importance of this topic, we should be particularly careful about clarifying its physical and conceptual foundations – both for ourselves and for our students. Unfortunately, the standard treatment of scattering (where the scattering particle is described as a plane wave, rather than a propagating, normalizable, finite-width wave packet) contains serious conceptual difficulties. In Section II we will briefly review the familiar plane wave approach to calculating reflection and transmission probabilities from a step potential and identify several conceptual problems that this approach presents.

In Section III, we present a novel alternative approach based on a straightforward analysis of the kinematics of wave packets which we believe provides a superior conceptual foundation for thinking about and introducing students to scattering. We thus demonstrate that many of the conceptual problems associated with the plane wave analysis (as well as some otherwise-pointless mathematical complications) can be quite simply avoided – all while preserving the mathematical simplicity and accessibility of the standard plane wave calculation.

A crucial implication of the proposed alternative ap-

proach is that standard plane wave calculations are *approximations* to realistic scattering events (where the relevant wave packet will always have finite spatial support). In order to illuminate this point, we illustrate, in the two subsequent sections, the relation between plane wave and wave packet treatments of scattering with two simple examples intended to illustrate two qualitatively different ways in which the plane wave analysis is imprecise or potentially misleading. In Section IV, we analyze the scattering of a Gaussian packet from a step potential, using this to develop a much more general exact expression for reflection and transmission probabilities. For this example, we show that the exact probabilities can be expanded in powers of the inverse packet width, with the individual terms analytically calculable. We thus show explicitly that the usual plane wave expressions for R and T emerge only in the limit of a very wide packet. In Section V we treat the reflection and transmission of a packet from a rectangular barrier and show that, in a certain limit, the plane wave treatment is not just slightly off, but instead badly misrepresents the qualitative behavior of the actual solution.

It may appear obvious to some readers that the standard plane wave analysis of scattering involves an approximation or idealization, and that, strictly speaking, scattering should always be thought of in terms of finite-width wave packets. However, most textbooks do not treat it as such. While some do discuss scattering in terms of wave packets^{1,2,3,4,5,6,7,8} (and see also References 9, 10, and Chapter 6 of 11), these tend to be more advanced texts. They also tend to present wave packets as a qualitative afterthought, with little discussion of the connection between the wave packets and the plane waves

that are, in the end, always used for actual calculations. Textbooks also often present wave packets in a misleading way – for example, by implying that wave packets merely provide a more physical and conceptually realistic way of re-deriving the really-correct plane wave expressions for R and T .¹ Further, these texts never clarify the nature of the approximation involved in the use of plane waves, nor do they address the domain of validity of this approximation; indeed, nearly all of these texts contain pictures of wave packets whose width is not much larger than the average incident wavelength and which (as we will show) are thus in fact very badly approximated by plane waves.

We note that in the vast majority of experimentally realizable situations, the wave packets are so wide (compared to other relevant length scales such as the de Broglie wavelength) that treating them as infinitely wide, i.e., as plane waves, is an excellent and appropriate approximation. Our concern is thus not with the correctness of the plane wave approach, but with the underlying conceptual and pedagogical issues: presenting scattering from the very beginning in terms of plane waves obfuscates what can and should be the clear connections between the formal calculations and the physical process of scattering, and hence pointlessly confuses students. It also obscures the fact that a plane wave treatment necessarily involves at least some degree of approximation. Hence our conclusion: it is in terms of wave packets that we should think about scattering ourselves, and introduce scattering to students.

II. THE PLANE WAVE ACCOUNT AND ITS PROBLEMS

Most students first encounter the quantum mechanical treatment of scattering with the simple example of a 1-D particle incident on a potential step:

$$V(x) = V_0 \theta(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } x > 0 \end{cases} \quad (1)$$

We will base our discussion on this example, although everything we will say can be applied to scattering problems in general (including 3D problems, where R and T are replaced by the differential cross section).

We begin this section with the familiar plane wave calculation of R and T probabilities for the potential step as it is presented in most textbooks.^{2,3,4,5,6,12,13,14,15} We then discuss the possible conceptual problems this approach presents for students. (See also Ref. 16 for research on related student difficulties with plane waves.)

The standard derivation begins by finding solutions to the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) + V(x) \psi(x) = E \psi(x) \quad (2)$$

valid on the two sides of the origin:

$$\psi_k(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{for } x < 0 \\ Ce^{i\kappa x} & \text{for } x > 0 \end{cases} \quad (3)$$

where $k^2 = 2mE/\hbar^2$ and $\kappa^2 = k^2 - 2mV_0/\hbar^2$. In principle the solution for $x > 0$ should be supplemented by an additional term: $De^{-i\kappa x}$. This term is omitted on the grounds that one is envisioning a particle incident from the left (the A term): it may reflect back toward the left (the B term) or transmit through to the right (the C term), but cannot be found on the right moving to the left.

Imposing the usual continuity conditions on ψ at $x = 0$ gives the following expressions relating the amplitudes of the incident, reflected, and scattered waves:

$$\frac{B}{A} = \frac{k - \kappa}{k + \kappa} \quad (4)$$

and

$$\frac{C}{A} = \frac{2k}{k + \kappa}. \quad (5)$$

The reflection (R) and transmission (T) probabilities are then given by

$$R = \frac{|C|^2}{|A|^2} = \left(\frac{k - \kappa}{k + \kappa} \right)^2 \quad (6)$$

and

$$T = \frac{\kappa}{k} \frac{|C|^2}{|A|^2} = \frac{4k\kappa}{(k + \kappa)^2}. \quad (7)$$

These expressions are often (though not exclusively) justified by reference to the *probability current*

$$j = \frac{-i\hbar}{2m} \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right). \quad (8)$$

which describes the flow of quantum mechanical probability.

For a wave or wave component with a plane wave structure, e.g., $\psi_A = Ae^{ikx}$, Equation (8) gives the probability current

$$j_A = \frac{\hbar k}{m} |A|^2 \quad (9)$$

and similarly for j_B and j_C . The plane wave probability current can also be understood as the probability density ($|A|^2$) multiplied by the group velocity

$$v_g(k) = \frac{d\omega(k)}{dk} = \frac{\hbar k}{m} \quad (10)$$

where $\omega(k) = E(k)/\hbar = \hbar k^2/2m$.

The reflection and transmission coefficients are given by the ratios of the individual probability currents for the reflected and transmitted terms to the incident current:

$$R = \frac{|j_R|}{j_I} \quad (11)$$

and

$$T = \frac{j_T}{j_I}. \quad (12)$$

Substituting Equation (9) and the analogous expressions for j_B and j_C into Equations (11)-(12) yields Equations (6)-(7).

While this approach appears concise, clear, and rigorously correct to a physicist who is already familiar with the concepts involved, it may be confusing to a student encountering scattering for the first time for several reasons.

First and foremost, the basic method of using the general solution to the time-independent Schrödinger equation is disconnected from the time-dependent intuitive picture that both physicists and students use to describe the physical situation of scattering: we say that particles propagate from the left, reflect or transmit at $x = 0$, and subsequently propagate out to the left or right. This description assumes a very specific physical situation, namely that of a wave packet approaching the step with some definite width, position, speed, and time. This physical picture is in play, tacitly, in the justification of several of the steps in the standard plane wave derivation. For example, the fact that particles *propagate* suggests the choice of complex exponentials rather than sines and cosines in Equation (3), and the fact that particles must begin in some specific location suggests the elimination of the D term. However, most textbooks do not make any explicit attempt to connect the plane wave expressions to the intuitive time-dependent physical picture described here. This invites a serious disconnect in the minds of students between the formal development and the physical process the formalism is supposed to be describing – i.e., it works against efforts to encourage students “to think of the problem statement as describing a physical process – a movie of a region of space during a short time interval...”¹⁷

A further conceptual problem is that certain aspects of Equations (6)-(7) are not intuitively clear. In particular, it is difficult to give an intuitive explanation for the factor of κ/k which enters in Equation (7). According to the standard probability interpretation of the wave function, R and T should be given by the area under the reflected and transmitted parts of $|\psi|^2$, respectively (assuming the wave function is normalized). Since these areas are infinite for plane waves, one can’t calculate that as one would naively expect. It is quite tempting (and quite wrong) to assume that the infinite widths simply cancel, giving $R = |B|^2/|A|^2$ and $T = |C|^2/|A|^2$ (without the factor of κ/k). We have observed that this is a common mistake among both physics students and teachers, but most textbooks do not confront it directly.

Textbooks explain the equations for R and T using one of the following approaches: (a) deriving Equations (6)-(7) using probability current^{2,3,4,5,6,12,13,14,15} as we sketched above, (b) giving these equations without explanation^{1,6}, (c) avoiding these equations altogether by

skipping the step potential and going straight to tunneling through a square barrier, using $T = |C|^2/|A|^2$ without mentioning that this happens to be correct only for the special case where the potential is equal on both sides of the barrier^{7,8,18,19,20,21}, or – perhaps most bizarrely – (d) stating that the factor of k in Equation (7) is due to “accepted convention” to ensure that $R + T = 1$.⁴

Approaches (c) and (d) are misleading and encourage an incorrect understanding that will lead students to errors when exposed to scattering in new contexts. Approach (b) does nothing to help students understand the meaning of these equations or apply them in other contexts. Approach (a) is generally considered the most correct and rigorous. But even this approach introduces difficulties for students. Probably current is an important concept that students need to learn, especially in an advanced course. However, it is a rather sophisticated concept, and it is introduced in the context of scattering, often for the first time, *solely* for the purpose of deriving R and T . Introducing such a concept in the middle of a derivation places extra cognitive load on students, increasing the likelihood that they will give up on understanding and just accept the results “on faith,” as magic formulas to be memorized and used without comprehension. Further, it is difficult to make a rigorous, rather than hand-waving, argument for why Equations (11)-(12) are the correct expressions for R and T in terms of probability current.

One advantage of the probability current approach is that it does give a somewhat intuitive explanation for the κ and k factors that appear in Equation (7): if the incoming and transmitted waves are traveling at different speeds, then it makes sense that the amount transmitted, and therefore the transmission probability, should be proportional to the ratio of the speeds, which are in turn given by Equation (10). However, this advantage is tempered by two problems. First, this explanation is difficult to relate to the standard probability interpretation and the intuition that the probability should be given by the area under the curve of $|\psi(x)|^2$. Second, it is not intuitively clear why the relevant speed should be the group velocity rather than the phase velocity. Indeed, it is not even clear what the group velocity means for a plane wave.²⁵ If one tries to gain an intuitive understanding of the formula for the transmission coefficient by looking at a simulation of plane waves incident on a step potential²⁶, one will actually be misled, since the only velocity that is apparent to the eye, the phase velocity, has a response to changes in potential that is opposite to that of the group velocity. That is, in a region where the potential is increased (like the $x > 0$ region of our step potential), the group velocity *decreases* whereas the phase velocity *increases*. The attempt to intuitively understand Equations (6) - (7) as ratios of speeds-times-intensities for the various wave components is thus likely to fail.

In summary, the standard analysis of 1-D scattering in terms of plane waves, although mathematically simple, obscures the inherently time-dependent physical nature

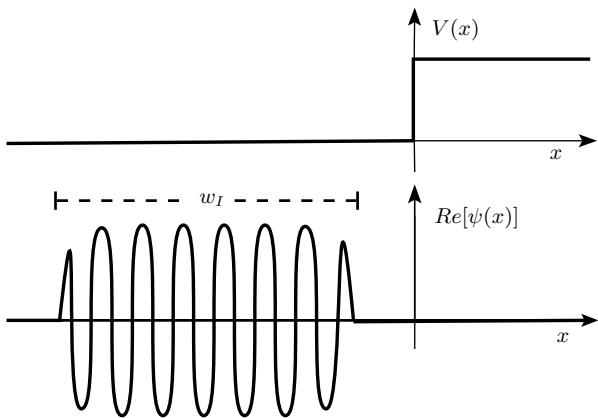


FIG. 1: A generic wave packet (with approximately-constant amplitude over most of its width, w_I) is incident on the step potential's scattering center at $x = 0$.

of scattering, requires a cognitive-load-increasing pedagogical detour through probability current (or dubious and misleading hand-waving, or obfuscation), and raises deep questions which are not easily answerable without stepping back from and getting underneath the plane wave approach. Wouldn't it be nice if there were some alternative approach that (a) didn't require the overhead of probability current and (b) required students to think, from the very beginning, that we are really dealing with propagating, finite-width *wave packets* to which the plane waves are merely a convenient *approximation*? Just such an approach will be presented in the following section.

III. SCATTERING PROBABILITIES AND PACKET WIDTHS

In this section we present an alternative derivation of the reflection and transmission probabilities that uses wave packets instead of plane waves. We recommend basing students' first introduction to scattering on this alternative approach. It is simpler than the standard plane wave derivation, builds on the standard $|\psi|^2$ definition of probability (rather than the more sophisticated idea of probability current), and provides a clear intuitive explanation for why the ratio of wave numbers (or equivalently group velocities) appears in the equation for the transmission coefficient.

Consider a wave packet approaching the scattering center at $x = 0$ for the potential defined in Equation (1), as indicated in Figure 1. Assume the packet has an almost-exactly constant amplitude (A) and wavelength ($\lambda_0 = 2\pi/k_0$) in the region (of width w_I) where the amplitude is non-vanishing, as shown in the Figure. Thus, where the amplitude is non-zero, the packet will at each moment be well-approximated by a plane wave:

$$\psi = A e^{ik_0 x}. \quad (13)$$

We may assume this incident packet is normalized, so

that $|A|^2 w_I = 1$.

What happens as the packet approaches and then interacts with the potential step at $x = 0$? To begin with, the packet retains its overall shape as it approaches the scattering center (that is, we assume that the inevitable spreading of the wave packet is negligible on the relevant timescales). It simply moves at the group velocity corresponding to the central wave number for the region $x < 0$:

$$v_g^< = \frac{\hbar k_0}{m}. \quad (14)$$

We then divide the scattering process into three stages:

- The leading edge of the packet arrives at $x = 0$
- The constant-amplitude “middle” of the packet is arriving at $x = 0$
- The trailing edge of the packet arrives at $x = 0$

Suppose the leading edge arrives at time t_1 . Then the trailing edge will arrive at t_2 satisfying

$$t_2 - t_1 = w_I / v_g^< = w_I m / \hbar k_0. \quad (15)$$

For intermediate times, $t_1 < t < t_2$, we will have, in some (initially small, then bigger, then small again) region surrounding $x = 0$, essentially the situation described in Equation (3), namely: a superposition of rightward- and leftward-directed plane waves (just to the left of $x = 0$) and a rightward-directed plane wave with a different wave number (to the right). And the same relations derived in the previous section for the relative amplitudes of these three pieces will still apply.

While crashing into the scattering center, the incident packet “spools out” waves – with amplitudes B and C given in Equations (4) and (5) – which propagate back to the left and onward to the right, respectively. These scattered waves will also be wave packets, with their leading and trailing edges produced at times t_1 and t_2 respectively.

This dynamical picture yields a very simple and illuminating alternative way to derive Equations (6)-(7), that is, the relations between the amplitude ratios (B/A and C/A) and the reflection and transmission probabilities. Consider first the reflected packet. The probability of reflection, R , is by definition just its total integrated probability density – which here will be its intensity $|B|^2$ times its width w_R . But the width of the reflected packet will be the same as the width of the incident packet: because these two packets both propagate in the same region, they have the same group velocity, so the leading edge of the reflected packet will be a distance w_I to the left of $x = 0$ when the trailing edge of the reflected packet is formed. Thus, we have

$$R = w_R |B|^2 = w_I |B|^2 = \left| \frac{B}{A} \right|^2 \quad (16)$$

where we have used the normalization condition for the incident packet: $w_I|A|^2 = 1$.

Similarly, the total probability associated with the transmitted wave will be its intensity $|C|^2$ times its width w_T . But w_T will be *smaller* than w_I because the group velocity on the right is slower than on the left. In particular: the leading edge of the transmitted packet is created at t_1 ; the trailing edge is created at t_2 ; and between these two times the leading edge will be moving to the right at speed

$$v_g^> = \frac{\hbar\kappa_0}{m} \quad (17)$$

where $\kappa_0^2 = k_0^2 - 2mV_0/\hbar^2$ is the (central) wave number associated with the transmitted packet. Thus, the width of the transmitted packet – the distance between its leading and trailing edges – is

$$w_T = v_g^> (t_2 - t_1) = \frac{\kappa_0}{k_0} w_I \quad (18)$$

and so the transmission probability is

$$T = w_T|C|^2 = \frac{\kappa_0}{k_0} \left| \frac{C}{A} \right|^2 \quad (19)$$

in agreement with Equation (7).

To summarize, one can derive the usual plane wave expressions for R and T merely by considering the kinematics of wave packets, without ever mentioning plane waves or probability current. Further, the perhaps-puzzling factor of κ_0/k_0 in the expression for T has an intuitive and physically clear origin in the differing *widths* of the incident and transmitted packets, which in turn originates from the differing group velocities on the two sides.

This route to the important formulas is both simpler and more physically revealing than the one traditionally taken in introductory quantum texts: there is a clearly defined initial condition and a definite process occurring in time; probability only enters in the standard way (as an integral of the probability density $|\psi|^2$); and the two quantities needed to define the probabilities (the packet widths and amplitudes) are arrived at separately and cleanly.

In addition, thinking in terms of wave packets can help students recognize that the formulas developed above for reflection and transmission probabilities (and this point applies equally well to three-dimensional scattering situations) are *approximations* and to understand when those approximations do and do not apply.

In particular, the argument presented here suggests that the mathematical expressions for R and T above will apply only in the limit of very wide incident packets. This has several aspects. First, we are justified in neglecting the dynamical spreading of the wave packet (and hence, e.g., treating the reflected packet as having the same width as the incident packet) only if the speed of spreading is very small compared to the group velocity, that is, if $\Delta k \ll k_0$, where $\Delta k \sim 1/\Delta x \sim 1/w_I$ is

the width of the incident packet in k -space. This implies that $w_I \gg \lambda_0$: the width of the wave packet should be much larger than the characteristic wavelength.

Second, the plane wave style derivation of the amplitudes assumes that, for some time interval (roughly, $t_1 < t < t_2$), the wave function's structure in some (variable) spatial region around $x = 0$ is indeed given by Equation (3). But these conditions will simply fail to apply if the actual wave function is (in the appropriate space and time regions) insufficiently plane wave-like, e.g., if the amplitude of the wave varies appreciably over a length scale $\lambda_0 = 2\pi/k_0$. Thus (assuming a smooth spatial envelope for the packet) the formulas will be valid in the limit $w_I \gg \lambda_0$, which is mathematically equivalent to the limit noted previously.

Third, the statements made above about the group velocities for the reflected and transmitted packets are not precisely true, because the reflected and transmitted packets need not be precisely centered (in k -space) about k_0 and κ_0 respectively. This is because the higher- k components of the incident packet are (typically) marginally more probable to transmit than the lower- k components (though the opposite behavior is also possible). Hence, the transmitted packet will (typically) peak around a value slightly greater than κ_0 , and the reflected packet will (typically) peak around a value slightly less than k_0 . These changes, however, will vanish for packets that have a narrow k -space distribution, i.e., a large width in physical space. (See Ref. 22 for an illuminating discussion of this “velocity effect.”)

Note finally that for a scattering center which has some finite width (e.g., a rectangular barrier), there is an additional length scale in the problem, and qualitative arguments also suggest that the plane wave type analysis should be valid only in the limit where the packet width is large compared to the spatial size of the scattering region: basically, the qualitative argument presented above (for the step potential, where scattering only occurs at $x = 0$) will go through unchanged only so long as the width of the region where scattering occurs (e.g., the width of a rectangular barrier) is much smaller than the packet width.

Even students who are just encountering quantum mechanical scattering for the first time should be able to understand all of these points (with the exception maybe of the third). That is, they should be able to understand how to think about scattering in terms of wave packets and how the standard textbook formulas (derived using plane waves) should be thought of as applying, as approximations, to wave packets that are wide compared to other length scales in the problem, e.g., λ_0 and the width of the scattering region.

The relevant length scale for the “velocity effect” mentioned above is the inverse of dT_k/dk , where T_k is the plane wave transmission probability for incident wave number k . Beginning students won't understand that. But this point overlaps with the more intuitively obvious point about the scattering width, and so can be simply

ignored. There are also some subtleties associated with the applicability of the group velocity concept; for example, the length scale over which the amplitude of the incident packet changes appreciably (roughly the width of the packet's edges) should also be (contrary to our Figure 1!) large compared to the central de Broglie wavelength.

We thus acknowledge that, like the plane wave approach we criticize, the approach outlined here has some subtle presuppositions which students may not grasp and which may conceivably lead to confusion and error. Nevertheless, we think the wave packet kinematics approach outlined here is far superior to the traditional derivations, in that it is fundamentally built around the time-dependent physical process of a scattering wave packet. It thus clarifies and highlights the essential physics, which the plane wave approach tends to obscure.

To emphasize the claims made in the preceding qualitative discussion, we include in the next two sections two more exact treatments of finite-width wave packets scattering from some typical textbook potentials. The main point is to concretize, with these two examples, the fact that the plane wave approximation is valid only when the packet width is large compared to all other physically relevant length scales.

IV. GAUSSIAN WAVE PACKET SCATTERING FROM A STEP POTENTIAL

It is possible to work out the *exact* R and T probabilities for a Gaussian wave packet incident on the potential step of Equation (1). Most of the derivation is worked out in several texts.^{1,2} But invariably these texts fail to write down the exact expressions for R and T and instead make last-minute approximations which result in the plane wave results developed previously. But it is worth pushing through the calculation to the end, if only to illustrate that the end exists and that the results reduce to the plane wave formulas *only in the appropriate limits*. Having the exact result in hand also allows one to analytically pick off explicit expressions for first non-vanishing corrections to the plane wave result, which is a great example calculation to share with students. That the corrections are small in precisely the limits discussed qualitatively at the end of the previous section, is also a nice confirmation of that discussion.

We begin with an incident Gaussian wave packet, with central wave number k_0 and width σ and centered, at $t = 0$, at $x = -a$:

$$\psi(x, 0) = (\pi\sigma^2)^{-1/4} e^{ik_0(x+a)} e^{-(x+a)^2/2\sigma^2}. \quad (20)$$

We then follow Shankar's text² and proceed in four steps.

Step 1 is to find appropriately normalized energy eigenfunctions for the step potential. These may be parametrized by k and are (up to normalization) just

the plane wave states given previously:

$$\psi_k(x) = \frac{1}{\sqrt{2\pi}} \left[\left(e^{ikx} + \frac{B}{A} e^{-ikx} \right) \theta(-x) + \frac{C}{A} e^{i\kappa x} \theta(x) \right] \quad (21)$$

where, as before, $\kappa^2 = k^2 - 2mV_0/\hbar^2$ and B/A and C/A are to be interpreted as the *functions of k* given by Equations (4) and (5). The overall factor of $1/\sqrt{2\pi}$ out front is chosen so that

$$\int \psi_{k'}^*(x) \psi_k(x) dx = \delta(k - k'). \quad (22)$$

We are here assuming that only eigenstates with energy eigenvalues $E = \hbar^2 k^2 / 2m > V_0$ will be present in the Fourier decomposition of the incident packet and hence we make no explicit special provision for those ψ_k for which κ is imaginary. (For a more rigorous treatment see Ref. 23; the approximations we introduce here don't change any of the central conclusions.) Note also that there are two linearly independent states for each E only one of which is included here. The orthogonal states will have incoming, rather than exclusively outgoing, plane waves for $x > 0$; such states will never enter given our initial conditions.

Step 2 is to write the incident packet as a linear combination of the ψ_k s:

$$\psi(x, 0) = \int \psi_k(x) \phi(k, 0) dk \quad (23)$$

where (assuming $\sigma \ll a$ so the amplitude of the incident packet vanishes for $x > 0$)

$$\phi(k, 0) = \left(\frac{\sigma^2}{\pi} \right)^{1/4} e^{-(k-k_0)^2 \sigma^2 / 2} e^{ika} \quad (24)$$

turns out to be the ordinary Fourier Transform of $\psi(x, 0)$.

Step 3 is to write $\psi(x, t)$ by appending the time-dependent phase factor to each of the energy eigenstate components of $\psi(x, 0)$:

$$\begin{aligned} \psi(x, t) &= \int \psi_k(x) \phi(k, t) dk \\ &= \int \psi_k(x) \phi(k, 0) e^{-iE(k)t/\hbar} dk \\ &= \left(\frac{\sigma^2}{4\pi^3} \right)^{1/4} \int e^{-i\hbar k^2 t / 2m} e^{-(k-k_0)^2 \sigma^2 / 2} e^{ika} \\ &\quad \times \left[e^{ikx} \theta(-x) + \left(\frac{B}{A} \right) e^{-ikx} \theta(-x) \right. \\ &\quad \left. + \left(\frac{C}{A} \right) e^{i\kappa x} \theta(x) \right] dk. \end{aligned} \quad (25)$$

We can then finally – Step 4 – analyze the three terms for physical content. The first term, aside from the

$\theta(-x)$, describes the incident Gaussian packet propagating to the right. For sufficiently large times (when the incident packet would have support exclusively in the region $x > 0$) the $\theta(-x)$ kills this term – i.e., the incident packet eventually vanishes.

The second and third terms describe the reflected and transmitted packets, respectively. If the factors (B/A) and (C/A) were constants, we would have Gaussian integrals which we could evaluate explicitly to get exact expressions for the reflected and transmitted packets – which would themselves, in turn, be Gaussian wave packets which could be (squared and) integrated to get exact expressions for the R and T probabilities. However, these factors are functions of k . It is not unreasonable to treat them as roughly constant over the (remember, quite narrow) range of k where $\phi(k, 0)$ has support. This is the approach taken by Shankar (and, at least by implication, several other texts) and the result is precisely the plane wave expressions for R and T we developed earlier.

But another approach (which, surprisingly, we have not found in the literature) is also appealing. Consider the second and third terms of Equation (25) – which represent (for late times when these terms are non-vanishing) the reflected and transmitted packets. These can be massaged to have the overall form (again assuming t sufficiently large that the θ factors can be dropped)

$$\psi_{R/T}(x, t) = \int \frac{e^{ikx}}{\sqrt{2\pi}} \phi_{R/T}(k, t) dk. \quad (26)$$

Putting the two terms in this form requires a change of variables – from k to $-k$ for the R term, and from k to $\sqrt{k^2 - 2mV_0/\hbar^2}$ for the T term. The resulting expressions for the k -space distributions of the reflected and transmitted packets are:

$$\phi_R(k, t) = \left(\frac{\sigma^2}{\pi}\right)^{1/4} e^{i\hbar k^2 t/2m} e^{-(k+k_0)^2 \sigma^2/2} e^{-ika} \left(\frac{k+\kappa}{k-\kappa}\right) \quad (27)$$

and

$$\begin{aligned} \phi_T(k, t) = & \left(\frac{\sigma^2}{\pi}\right)^{1/4} e^{-i\hbar(k^2+2mV_0/\hbar^2)t/2m} e^{-(\sqrt{k^2+2mV_0/\hbar^2}-k_0)^2 \sigma^2/2} \\ & \times e^{ika} \left(\frac{2\sqrt{k^2+2mV_0/\hbar^2}}{\sqrt{k^2+2mV_0/\hbar^2}+k}\right) \frac{k}{\sqrt{k^2+2mV_0/\hbar^2}}. \end{aligned} \quad (28)$$

To find the total probability associated with a given packet, we can just as well integrate the momentum-space wave functions as the position-space wave func-

tions. Thus,

$$\begin{aligned} R &= \int |\phi_R(k, t)|^2 dk \\ &= \left(\frac{\sigma^2}{\pi}\right)^{1/2} \int e^{-(k+k_0)^2 \sigma^2} \left(\frac{k+\kappa}{k-\kappa}\right)^2 dk \\ &= \left(\frac{\sigma^2}{\pi}\right)^{1/2} \int e^{-(k-k_0)^2 \sigma^2} \left|\frac{B}{A}\right|^2 dk \end{aligned} \quad (29)$$

where in the last step we have done another change of variables from k to $-k$. This result can be summarized as follows:

$$R = \int P(k) R_k dk \quad (30)$$

where $P(k) = |\phi(k, 0)|^2$ is the probability density for a given k associated with the incident packet, and R_k is simply the reflection probability for a particular value of k as expressed in Equation (6).

The analogous result for the T term emerges after some more convoluted algebra:

$$\begin{aligned} T &= \int |\phi_T(k, t)|^2 dk \\ &= \left(\frac{\sigma^2}{\pi}\right)^{1/2} \int e^{-(\sqrt{k^2+2mV_0/\hbar^2}-k_0)^2 \sigma^2} \\ &\quad \times \left(\frac{2\sqrt{k^2+2mV_0/\hbar^2}}{\sqrt{k^2+2mV_0/\hbar^2}+k}\right)^2 \frac{k^2}{k^2+2mV_0/\hbar^2} dk \\ &= \left(\frac{\sigma^2}{\pi}\right)^{1/2} \int e^{-(k-k_0)^2 \sigma^2} \left|\frac{C}{A}\right|^2 \frac{\kappa}{k} dk \\ &= \int P(k) T_k dk. \end{aligned} \quad (31)$$

where in the next-to-last step we have made a change of variables (back!) from k to $\sqrt{k^2+2mV_0/\hbar^2}$.

These expressions are exact (subject to the assumptions noted earlier). Note that, if we treat $|B/A|^2$ and $(\kappa/k)|C/A|^2$ as constants that do not depend on k (i.e., if we approximate these functions by their values at $k = k_0$, which is a good approximation so long as the functions don't vary appreciably in a region of width $1/\sigma$ around k_0 , i.e., if the width σ of the incident packet is very big) we are left with plain Gaussian integrals that can be evaluated to get back the plane wave-approximation results we started with: $R = |B/A|^2$ evaluated at $k = k_0$, etc.

Unfortunately, the actual integrals are too messy to do exactly. But we can Taylor expand the complicating factors around $k = k_0$ to get a series of standard integrals, resulting in a power-series expansion (in inverse powers of the packet width σ) for the exact R and T .

The first two non-vanishing terms for R and T are as follows:

$$R = \left(\frac{k_0 - \kappa_0}{k_0 + \kappa_0}\right)^2 + \left(\frac{2k_0}{\kappa_0^3} + \frac{8}{\kappa_0^2}\right) \left(\frac{k_0 - \kappa_0}{k_0 + \kappa_0}\right)^2 \frac{1}{\sigma^2} + \dots \quad (32)$$

and

$$T = \frac{4k_0\kappa_0}{(k_0 + \kappa_0)^2} - \left(\frac{2k_0}{\kappa_0^3} + \frac{8}{\kappa_0^2} \right) \left(\frac{k_0 - \kappa_0}{k_0 + \kappa_0} \right)^2 \frac{1}{\sigma^2} + \dots \quad (33)$$

The first terms are just the standard plane wave results. The leading-order corrections vanish (roughly) in the limit $\sigma^2 k_0^2 \gg 1$, which confirms the conclusion of the qualitative discussion in Section III: the plane wave approximation will be accurate only if the packet width is very large compared to the de Broglie wavelength, $\lambda_0 = 2\pi/k_0$.

Note also that Equations (30)-(31) hold much more generally than just for Gaussian wave packets and step potentials. One can assume an arbitrary initial wave packet with k -space distribution $\phi(k, 0)$ and arbitrary potential function $V(x)$ (subject to the assumption that it is asymptotically constant on both sides of the scattering region), and still carry through the above derivation. One cannot say much in general about R_k and T_k for an arbitrary potential, but Equations (30) - (31) will still hold.

V. SCATTERING FROM A RECTANGULAR BARRIER

In the previous section we showed that, for scattering from a step potential, the standard textbook formulas are approximations which are increasingly correct as the width of the incident packet is taken to infinity. We now turn to a different example – scattering from a rectangular barrier – to show more explicitly something else we claimed earlier: if the scattering region has a finite width that is not small compared to the width of the incident packet, the plane wave approximation will give badly misleading, qualitatively wrong results.

Consider the potential barrier given by

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & 0 \leq x \leq a \\ 0 & x > 0. \end{cases} \quad (34)$$

For a packet that is narrow compared to the barrier width a , but still wide enough that we can ignore its dynamical spreading during the time interval of the collision, there is an elegant kinematical argument that allows one to work out the total reflection and transmission probabilities. See Figure 2. Following the principle (sometimes attributed to Wheeler) of never calculating anything until one already knows the result, we sketch this argument first.

For this argument, and the calculations that follow, we make several assumptions. First, we assume that the barrier is much wider than the wave packet, that is, $a \gg w$ or $\Delta k \gg 1/a$, where $w \sim 1/\Delta k$ is the width of the packet. This approximation ensures that we can treat the interaction of the packet with each side of the barrier independently. Second, we assume that the wave packet is wide

compared to its central wavelength $\lambda_0 = 2\pi/k_0$, that is, $w \gg \lambda_0$ or $k_0 \gg \Delta k$. This ensures that the packet does not spread out too much, and warrants making a plane wave approximation in treating the interaction of the packet with each edge of the barrier. Finally, we assume that $k_0 \gg \sqrt{2mV_0}/\hbar$, or $E \gg V_0$. This is not strictly necessary, but allows us to simplify the calculations by taking the reflection coefficient to be small.

Here's the kinematical argument. When the packet arrives at the left side of the barrier, there is probability R_{k_0} for it to reflect, where the R_{k_0} here (and the T_{k_0} to follow) is the probability for reflection (transmission) *from a step*. The packet may also transmit, then reflect off the step on the far side of the barrier, then transmit back out to the left: this has overall probability $T_{k_0} R_{k_0} T_{k_0}$. Similarly, it could reflect 3, 5, or any higher odd number of times inside the barrier before finally leaving to the left. (Note that R_{k_0} and T_{k_0} are the same whether one is going “up” or “down” the step.) The total probability of reflection is equal to the sum of all these possibilities (which are non-interfering so long as the packet remains narrow compared to the distances between adjacent packets):

$$\begin{aligned} R_{k_0}^{(\text{total})} &= R_{k_0} + T_{k_0} R_{k_0} T_{k_0} + T_{k_0} R_{k_0}^3 T_{k_0} + \dots \\ &= 2R_{k_0}/(1 + R_{k_0}) \end{aligned} \quad (35)$$

where we have summed a geometric series and used the fact that $R_{k_0} + T_{k_0} = 1$.

In the limit that $E \gg V_0$, we have $R_{k_0} \ll 1$, and Equation (35) reduces to

$$R_{k_0}^{(\text{total})} = 2R_{k_0}. \quad (36)$$

What happens if we instead calculate the reflection probability in the standard textbook way – namely, using the energy eigenstates of the Schrödinger equation to read off the reflection probability according to $R = |B/A|^2$? That is, what if we use the plane wave approximation? We will not repeat this calculation, as it can be found in many quantum mechanics textbooks,¹ but simply quote the result for the total reflection probability for a barrier potential:

$$R_{k_0}^{(\text{total})} = \left| \frac{B}{A} \right|^2 = \frac{(k_0^2 - \kappa_0^2)^2 \sin^2(\kappa_0 a)}{4k_0^2 \kappa_0^2 + (k_0^2 - \kappa_0^2) \sin^2(\kappa_0 a)} \quad (37)$$

where A and B are the amplitudes of the incident and reflected plane waves, respectively. Rewriting in terms of the reflection and transmission coefficients for the step potential, R_{k_0} and T_{k_0} , from Equations (6) and (7), gives:

$$R_{k_0}^{(\text{total})} = \frac{4R_{k_0} \sin^2(\kappa_0 a)/T_{k_0}^2}{1 + 4R_{k_0} \sin^2(\kappa_0 a)/T_{k_0}^2}. \quad (38)$$

As before, because $R_{k_0} \ll 1$, we may simplify this to:

$$R_{k_0}^{(\text{total})} = 4R_{k_0} \sin^2(\kappa_0 a) \quad (39)$$

where, just to be clear, the left-hand-side refers to the overall reflection probability from the rectangular barrier

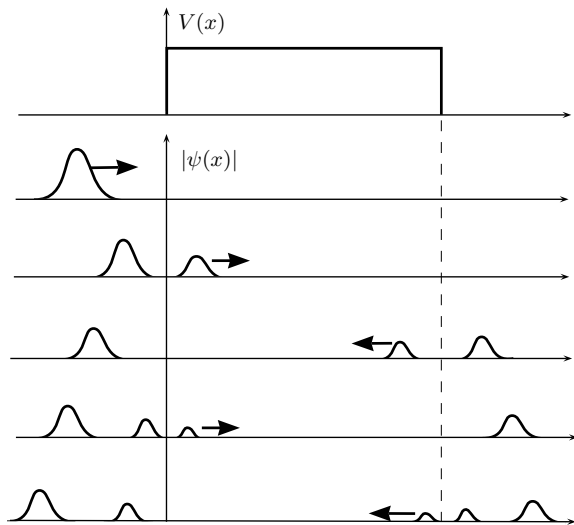


FIG. 2: The top frame shows $V(x)$ for the rectangular barrier. Subsequent frames show how $|\psi(x)|$ evolves in time for a wave packet incident from the left, through an infinite sequence of back-and-forth reflections inside the barrier. Note that the sizes of reflected packets are exaggerated relative to transmitted packets, compared to the assumptions made in the text.

and the R_{k_0} on the right hand side denotes the probability for reflection from a corresponding step potential, which is convenient since we want to compare with Equation (36).

This is the standard plane-wave approximation for the k_0 -dependent reflection probability from a rectangular barrier (for large E). Note in particular that – unlike the result of the kinematical argument sketched above – it oscillates rapidly back and forth between zero and $4R_{k_0}$ as k_0 varies, with a period of order $1/a$. So, if we believe the kinematical argument, we can already see a major qualitative disagreement between the reflection probability given by Equation (36), calculated using wave packets, and Equation (39), calculated from the plane-wave approximation.

The rigorous way to calculate the reflection probability for our wave packet is to use Equation (30). Part of the setup here was the assumption that the packet width was small compared to the width of the barrier, i.e., that Δk – the width of the packet in k -space – is large compared to $1/a$. This implies that the plane-wave result, Equation (39) will oscillate back and forth between its minimum and maximum values *many times* over the support of $P(k)$. And so the total reflection probability will simply be the average value of the plane-wave result:

$$R_{k_0}^{(\text{total})} = 2R_{k_0} \quad (40)$$

in agreement with Equation (36), the result of the kinematical argument.

Whereas the plane wave approximation predicts that the reflection probability rapidly oscillates between 0 and

$4R_{k_0}$, the actual probability is just $2R_{k_0}$ – insensitive to the precise value of k_0 . (The related oscillatory behavior of R as the width of the barrier is varied is displayed in Figure 10 of Ref. 22, which treats scattering in terms of wave packets. However, this figure shows only barrier widths that are smaller than the packet width. Yet, interestingly, it is suggested by the figure that the oscillations disappear as the barrier width approaches the packet width, which is consistent with our claims here.)

In addition to showing how the plane-wave approximation can give qualitatively wrong results when it is applied inappropriately, this example helps illustrate the useful generality of Equation (30) for the reflection coefficient. As the earlier step potential example showed, this formula correctly predicts the behavior in situations where the incoming wave packet is wide compared to the barrier (i.e., it reduces to the plane wave result in the appropriate limit). But as the rectangular barrier example shows, it also correctly predicts the behavior in situations where the incoming wave packet is small in comparison to some other length scale in the problem such that the plane wave approximation badly fails to capture the true, qualitative behavior of R .

VI. CONCLUSIONS

The standard introductory textbook presentations of quantum mechanical scattering are almost always in terms of unphysical plane wave states. After reviewing some of the conceptual problems and mathematical overhead of the plane wave approach, we showed in Section III how these problems can be largely avoided by instead deriving the basic expressions for reflection and transmission probabilities from a simple analysis of the kinematics of wave packets. This allows students to genuinely understand the connection between the formal calculations and the physical process of scattering, and hence encourages visualization and physical thinking (e.g., about relative length scales in the problem). In addition, the several (overlapping) approximations which enter into the analysis can be understood intuitively even by beginning students, which should help them understand that the R and T coefficients they encounter in textbooks (and homework problems) are *approximations* which are valid only in the limit of very wide packets.

To highlight the approximate character of the standard plane wave results, we computed exact expressions for R and T for a Gaussian wave packet incident on a step potential. We showed that these can be written in the suggestive (and, as it turns out, general) form of Equations (30) - (31). In the limit of very wide packets, these reduce to the plane wave results; close to that limit, it is possible and illuminating to use these formulas to generate a power series in the inverse packet width. This underscores the point that the plane wave approximation can be – and, in virtually all actual experimental situations, *is* – very accurate.

We then briefly discussed reflection and transmission from a rectangular barrier, such that the packet width is large compared to the central wavelength, but small compared to the width of the barrier. We showed explicitly that the plane wave approximation badly mischaracterizes the dependence of R and T on the central wave number k_0 , whereas Equations (30) - (31) handle everything automatically and correctly. This illustrates the general fact that the validity of the plane wave approximation relies on the packet width being large, not only compared to the central de Broglie wavelength, but large also compared to other length scales in the problem.

In addition to the pedagogical value of introducing scattering in terms of wave packets from the very beginning, our main conclusion is the importance and fundamentality of Equations (30) - (31), which we have never seen in any undergraduate quantum mechanics texts and have in fact seen only very rarely in the literature. (See, for example, References 22 and 24 and further references therein. Ref. 9 seems to mention the result in words without writing out the corresponding equations.)

It seems likely that the reason for this is that most physicists would regard these expressions as *obvious*. An incident wave packet is, after all, merely a superposition of plane wave states with some associated wave number probability distribution $P(k)$, and the reflection and transmission probabilities R_k and T_k can be defined individually for those states. So it seems almost irresistible to conclude that Equations (30) - (31) should be the right

expressions.

But we don't think it is so obvious. It cannot be so quickly taken for granted that "the reflection and transmission probabilities R_k and T_k can be defined" for the plane wave states. As we have discussed at length in Section II, standard derivations of R_k and T_k are really inconsistent, in that they presuppose a physical process that simply is not described by the posited mathematics. Simply put, plane waves do not reflect or transmit. The coefficients R_k and T_k are really only meaningful if thought of the way we've advocated here – as probabilities for the reflection and transmission of wave packets, in the limit where the packet width approaches infinity.

In short, it is the plane wave expressions that conceptually presuppose wave packets, not vice versa. It is thus a mistake to think that Equations (30) - (31) are trivially derivable from more basic, independently meaningful things. If anything, it is a surprise that the probabilities can be written in this form. But they can, and this should be more widely known. As should the general perspective which gave rise to them: thinking about scattering in terms of wave packets.

Acknowledgements:

Thanks to Mike Dubson and two anonymous referees for a number of helpful comments on earlier drafts.

-
- ¹ C. Cohen-Tannoudji, B. Diu, and F. Laloë, *Quantum Mechanics* (John Wiley, New York, 1977).
 - ² R. Shankar, *Principles of Quantum Mechanics* (Springer, 1994).
 - ³ A. P. French and E. F. Taylor, *An Introduction to Quantum Physics* (Norton, New York, 1978).
 - ⁴ R. Eisberg and R. Resnick, *Quantum Physics of Atoms, Molecules, Solids, Nuclei, and Particles* (John Wiley and Sons, New York, 1985).
 - ⁵ R. W. Robinett, *Quantum Mechanics; Classical Results, Modern Systems, and Visualized Examples* (Oxford University Press, New York, 1997).
 - ⁶ P. A. Tipler and R. A. Llewellyn, *Modern Physics* (W.H. Freeman and Company, New York, 2002), 4th ed.
 - ⁷ H. C. Ohanian, *Modern Physics* (Prentice, Englewood Cliffs, NJ, 1995), 2nd ed.
 - ⁸ D. J. Griffiths, *Quantum Mechanics* (Pearson, Upper Saddle River, 2005), 2nd ed.
 - ⁹ R. K. Hobbie "A simplified treatment of the quantum-mechanical scattering problem using wave packets", *Am. J. Phys.* **30**, 857 (1962).
 - ¹⁰ W. E. Gettys "Potential scattering of a wave packet", *Am. J. Phys.* **33**, 485 (1965).
 - ¹¹ R. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966).
 - ¹² A. Beiser, *Concepts of Modern Physics* (McGraw Hill, 2003), 6th ed.
 - ¹³ R. Harris, *Nonclassical Physics* (Pearson, 1998), 1st ed.
 - ¹⁴ L. D. Landau and L. M. Lifshitz, *Quantum Mechanics* (Elsevier, Oxford, 1977), 3rd ed.
 - ¹⁵ A. Goswami, *Quantum Mechanics* (Wm. C. Brown, Dubuque, 1997), 2nd ed.
 - ¹⁶ S. B. McKagan, K. K. Perkins, and C. E. Wieman "A deeper look at student learning of quantum mechanics: the case of tunneling", *Phys. Rev. ST: PER* **4**, 020103 (2008).
 - ¹⁷ A. V. Heuvelen "Learning to think like a physicist: a review of research-based instruction strategies", *Am. J. Phys.* **59**, 891 (1991).
 - ¹⁸ J. R. Taylor, C. D. Zafiratos, and M. A. Dubson, *Modern Physics for Scientists and Engineers* (Pearson Prentice Hall, Upper Saddle River, 2004), 2nd ed.
 - ¹⁹ K. Krane, *Modern Physics* (John Wiley and Sons, New York, 1996), 2nd ed.
 - ²⁰ R. A. Serway, C. J. Moses, and C. A. Moyer, *Modern Physics* (Saunders College Publishing, 2005), 1st ed.
 - ²¹ R. Knight, *Physics for Scientists and Engineers* (Pearson, San Francisco, 2004), 1st ed.
 - ²² M. H. Bramhall and B. M. Casper "Reflections on a wave packet approach to quantum mechanical barrier penetration", *Am. J. Phys.* **38**, 1136 (1970).
 - ²³ C. Hammer, T. Weber, and V. Zidell "Time-dependent scattering of wave packets in one dimension", *Am. J. Phys.* **45**, 933 (1977).
 - ²⁴ P. L. Garrido, S. Goldstein, J. Lukkarinen, and R. Tumulka "Paradoxical reflection in quantum mechanics", arXiv:quant-ph/0808.0610 (????).

²⁵ The best and only way we know to think about group velocity for a plane wave is to imagine the plane wave as a very wide packet. The group velocity is then the velocity

at which the entire packet moves.
²⁶ e.g. <http://phet.colorado.edu/tunneling>